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Calculating Sputter Rate Angular Dependence Using Optical Profilometry
PREPRINT

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Abstract: This work attempts to determine angular dependence curves for sputter rates of a material based on a single experimental measurement. An aluminum cylinder was exposed to a BHT-200 plume and the resulting erosion profile was measured. This profile was fed into an optimizer, which calculated the angular dependence curve to match the given erosion profile. The calculated profile matched well with the experimental profile, however neither matched well will previously published results. The likely cause of this discrepancy was the non-uniformity of the ion source used. As a further validation of the optimization routine, the angular dependence curve was input to the Coliseum plasma modeling code, which generated the same erosion profile as the experimental data.

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Nomenclature

Y	= sputter yield
E	= incident ion energy
$Q, \alpha^*, \Sigma, s, f, \theta_{opt}$	= empirical sputter curve fit parameter
M_1	= ion mass
M_2	= surface particle mass
S_n	= nuclear stopping power
U_s	= sublimation energy
Γ	= mechanism B-sputtering contribution
k_e	= Lindhard electronic stopping coefficient
ϵ	= reduced energy
dx	= erosion depth
Φ	= particle flux
N_A	= Avagadro's number
ρ_s	= surface material density
T	= time multiplier

I. Introduction

Surface sputtering and erosion are of paramount concern for missions utilizing electric propulsion (EP) based thrusters. Typical ion energies from EP thrusters can be in the hundreds of eV. Impingement of ions on a surface can cause substantial sputtering of the surface material. Surface sputtering can cause deposition onto optics, degradation of thermal systems, changes to electrical properties, and, in some cases, structural deformation. Several previous works have focused on single event ion sputtering and prediction. Boyd[1] presents a literature review of the current state of sputter prediction. Surface sputtering is highly dependent on the incident ion impact angle, and will therefore change over time as a given surface erodes. This work presents a new method for calculating the angular dependence of the sputter yield based on the erosion profile of a known reference cylinder.

A 0.25 inch aluminum cylinder was exposed to a BHT-200 plume for a period of 72 hours. The erosion profile was then measured using an optical profilometer. A computational optimizer was used to calculate the angular dependence of the sputter yield curve. To validate this angular dependence, the Coliseum plasma modeling package was then used to replicate the profile of the eroded cylinder.

Coliseum[2] is a framework consisting of several plasma simulation packages developed by the Air Force Research Lab, Advatech Pacific, and several universities and industries. This paper focuses on the Draco[3] package, a fully kinetic/hybrid ES-PIC routine. Draco utilizes a stretched Cartesian volume mesh intersected by a triangulated surface mesh. An erosion module has been added to the Draco code allowing for surface sputtering, redeposition, and the deformation of a surface over long time intervals.

Draco surfaces are composed of triangulated meshes. As particles impact a surface element, a sputter yield value is calculated and weighed onto each of the three nodes making up the element. At a user specified interval, the nodes are moved according the the accumulated erosion value. Nodes are moved along normal vectors formed by averaging the normal direction of all adjacent surface elements.

II. Experimental Setup

These experiments were conducted in Chamber 6 located at the Air Force Research Laboratory (AFRL) Electric Propulsion Laboratory located at Edwards AFB, CA. Chamber 6 measures 1.8 m in diameter and 3.0 m in length with a pumping speed of 32,000 l/s of xenon using four single stage cryopanels and one 50 cm dual stage cryopump. During nominal chamber operations chamber pressure is approximately 6×10^{-6} Torr, corrected for xenon.

The Busek Co, Inc. BHT-200 xenon Hall thruster was used in this experiment. The BHT-200 produces 12 mN of thrust at a system efficiency of 35% while operating at nominal discharge voltages and conditions, see Table 1.

For the purpose of this experiment, an aluminum alloy 6061 rod measuring 0.25 inches in diameter was used. Prior to plume exposure the rod was sandblasted to ensure a uniform surface texture and remove any oxidation. An 16 mm test section was identified for plume impingement. Adjacent to this section, Kapton tape was wrapped around the rod to protect a small area of the rod from the plume and provide a ready reference to measure the quantity of material eroded.

Optical profilometry measurements were performed to establish a pre-erosion baseline. The profilometer used was a STIL Micromeasure measurement system with a STIL CHR contactless optical sensor capable of 1 micron resolution. The available profilometry software cannot control a rotation stage, so a series of planar scans were taken in 30° increments controlled by a manual rotation stage.

The long axis of the rod was placed perpendicular to the thruster 10.7 cm downstream of the nose cone and aligned 90° to the thruster. In addition the rod was grounded to the chamber to prevent a localized charge buildup and sheathing effects. The rod was exposed to the thruster plume for a period of 72 hours. At the termination of the period the rod was again removed and profiled. The profilometry and chamber setups are shown in Figure 1.

III. Algorithms

A. Erosion

Surface erosion is calculated using the sputter yield and particle flux to a surface. Surface nodes are moved at user defined intervals based on the accumulated sputter. The sputter yield from the experimental results

Anode Flow	840 μg/s (Xe)
Cathode Flow	98 μg/s (Xe)
Anode Potential	250 V
Anode Current	0.85 A
Heater Current	3.0 A
Keeper Current	0.5 A
Magnet Current	0.75 A

Table 1. Nominal Operating Conditions: ***Typical operating conditions of the Busek BHT-200 Hall thruster.***

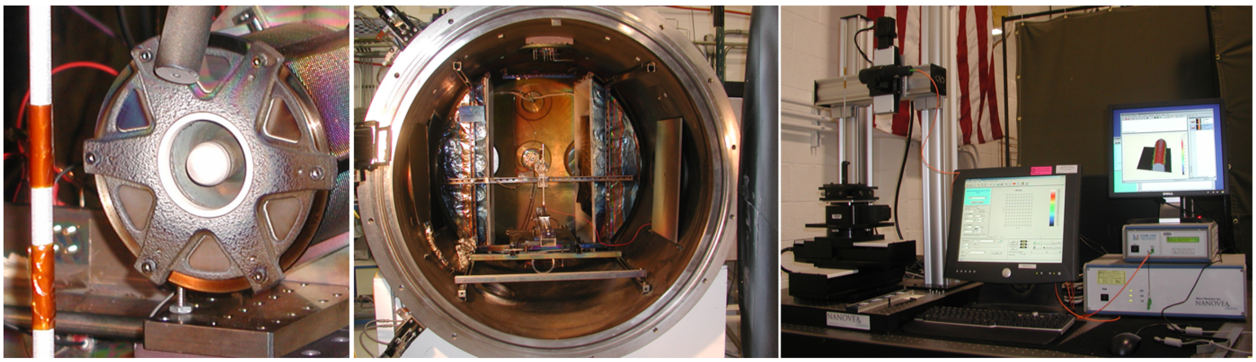

Figure 1. Aluminum rod and thruster in chamber (left and center). Profilometer with mounted rod (right).

was obtained by converting a distance into an molecular sputter yield.

$$dx = \frac{Y\Phi M_2}{N_A \rho_s} T \tag{1}$$

where Φ is the particle flux, M_2 is the molecular mass of the surface material, and ρ_s is the density of the surface material. For a typical plasma simulation, erosion rates are on a much larger timescale than plasma parameters. For this reason, a time multiplier, T, is applied to the erosion rate.

B. Sputter Yield

There are several algorithms to calculate sputter yield. This study used the Yamamura yield model. The Yamamoura normal yield is given by

$$Y(E) = 0.042 \frac{Q\alpha^*(M_2/M_1)Sn(E)}{U_s(1+\Gamma k_e \epsilon^{0.3})} \times \left[1 - \sqrt{\frac{E_{th}}{E}}\right]^s \tag{2}$$

where E is the incident energy and all other terms are material constants and empirical fit factors. Yamamura[5] presents a complete explanation and derivation of terms. For this study, an average normal yield was obtained using average flux and measured erosion at normal incidence. This average normal yield was then given as an input to the optimizer. The Yamamura angular dependance[6] is given by

$$Y(\theta) = Y(0)\cos^{-f}\theta e^{-\Sigma(\cos^{-1}\theta - 1)} \tag{3}$$

The optimum sputter angle then relates Σ and f.

$$\cos(\theta_{opt}) = \frac{\Sigma}{f} \tag{4}$$

C. Determination of Sputter Yield Angular Dependance

Given an eroded cylinder profile, the angular sputter yield dependence and normal sputter yield of the material can be determined. As shown in Equation 3, the angular dependence of the sputter yield for a given material and incident particle flux can be determined by two constants: f and Σ. An optimizer can be used to determine these constants by matching calculated erosion profiles with a measured experimental profile. A code was written to deform a cylinder over time using the Yamamura sputter yield. A uniform, monoenergetic flux was assumed. After a user specified time, the resulting profile is compared to a given profile using a least squares method for a variety of input states. This process is repeated with increasingly fine input resolution and narrow input range until an optimum solution is reached.

IV. Experimental Results

A 0.25 in aluminum cylinder was placed in a BHT-200 plume and allowed to erode for a period of 72 hours. The resulting surface profile was measured with an optical profilometer and compared to the initial profile. The resulting change in profile was fed into an optimizer and Yamamura constants were calculated to match the erosion rates attained.

The eroded cylinder is shown in Figure 2. Figures 3 and 4 show the measured profile. The degree increments correspond to the measured profiles in Figure 5 and the millimeter increments correspond to the measured profiles in Figure 6.

Figure 2. Aluminum rod before exposure (left) followed by 72 hour erosion photos ranging from -90 degrees to +90 degrees from incidence.

Figure 5 shows the erosion profile after 72 hours. The profiles are non-uniform due to a non-ideal plasma

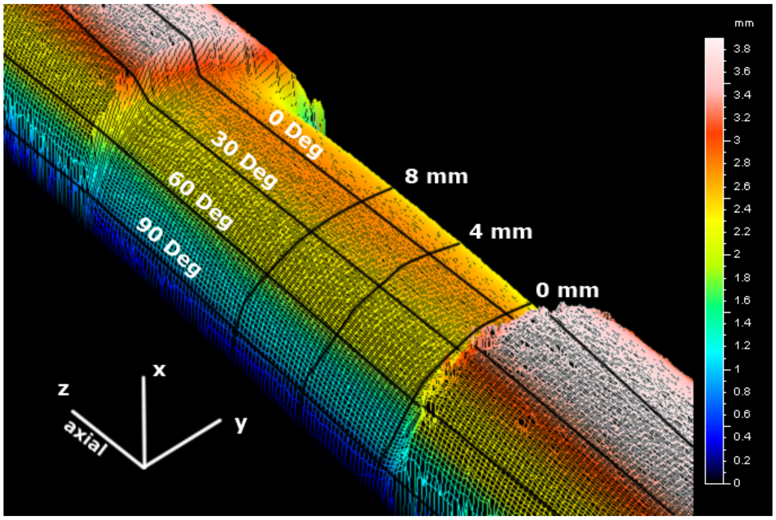

Figure 3. Erosion profile at normal incidence after 72 hours. Lines are shown as reference for future plots.

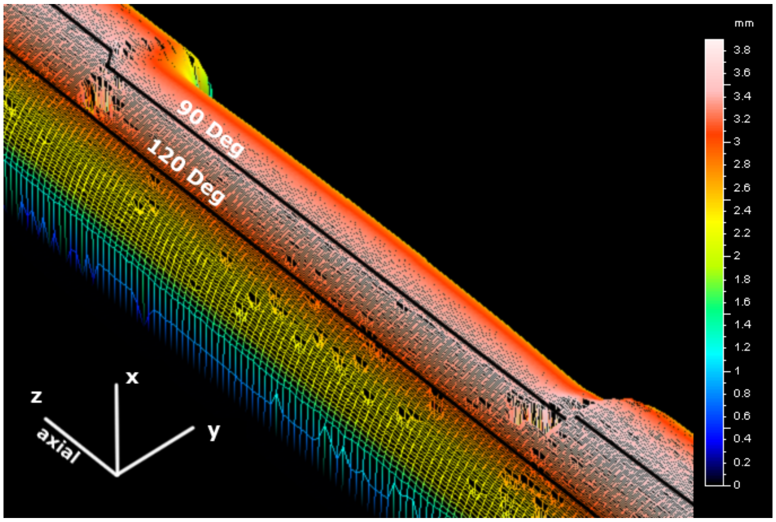

Figure 4. Erosion profile at 90° from incidence after 72 hours. Lines are shown as reference for future plots.

environment. There is a central bulge indicating less erosion near the center (8 mm) than near the taped area (0 mm). This may be because the tape itself affected the plasma. Kapton is a dielectric and may have charged to a non-zero potential. A potential gradient near the taped area could have accounted for a variable particle flux along the length of the exposed area.

There is also a higher erosion level towards the left side (0 mm, see Fig. 6) of the exposed area. This is likely due to the rod not being perfectly aligned with the centerline of the thruster. The exposed area was placed as close to the centerline of the thruster as was possible, but this does not guarantee alignment in the plume.

Thruster plumes are not always focused directly over the centerline and there may have been a small rotation in the thruster mounting causing off-center impingement. Significant erosion is shown to have occurred at 90° and a small amount of erosion as far as 120°. This is due to the overall erosion of the surface. As the surface erodes, the point on the surface at 90° from the thruster is no longer the point of maximum horizontal distance. This is shown in Figure 4.

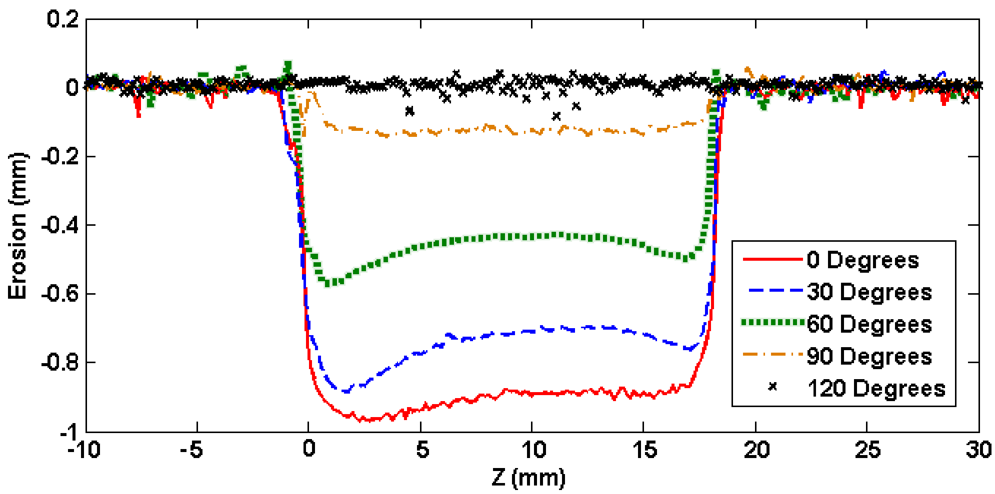

Figure 5. Erosion profile in the axial direction at varying positions on the rod (See Fig. 3).

The cross sectional erosion profile is shown in Figure 6 along with the average total erosion over the three measurements and the baseline, uneroded profile. A slight non-uniformity is present. The profile near the taped area has a higher erosion rate at higher angles and a lower erosion rate near normal incidence than the centerline (0 degree) profile. Again, this may have been caused by effects related to the Kapton tape. This nonuniformity is shown more clearly in Figure 7.

The centerline (8 mm) profile was input to the optimizer and Yamamura constants were determined for the described erosion profile. A resulting contour plot of the error in the least squares fit is shown in Figure 8. For graphical reasons, the maximum value was capped at 100 and undefined values are shown as 0. A line of local minima is present in the contour. This line represents a profile where the normal erosion and the high angle erosion are the most accurate. As the line of local minima itself lowers to an absolute minimum, the erosion profile begins to match more closely in the intermediate angle value range. For this case, optimum values were found to be 1.1 for f and 0.1 for Σ.

The calculated values for f and Σ did not match the expected values. Based on published material and empirical constants, aluminum exposed to 200 eV ions should have an f of 8.6 and a Σ of 4.3. In Figure 8 these values would lie in the bottom of the trough representing local minima, however would not be the absolute minimum. This implies that the erosion near 0 and 90 degrees is correct, however the intermediate values are not correct.

As points move down the line of local minima towards a Σ value of 0, the erosion profile becomes more circular with a weaker angular dependancy for small angles and a larger angle dependency at high angles. Larger values tend to have a stronger angular dependency at smaller angles. This difference is shown in Figure 9. The published Yamamura constants for aluminum yield a dependence curve with a maximum yield around 60°. The calculated constants represent a maximum yield of similar magnitude, but at 80°. A flatter dependence curve, or one where the peak is at a high angle, will result in a relatively uniform erosion

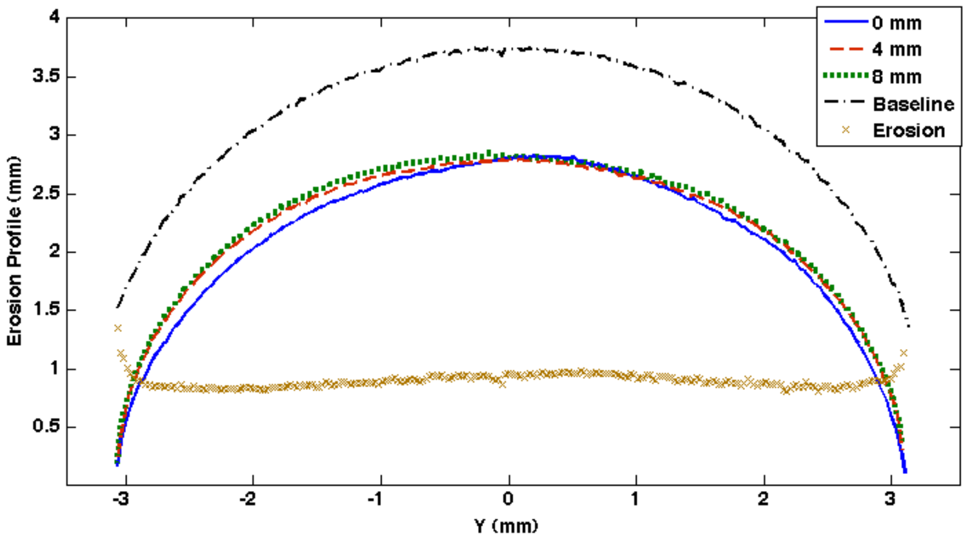

Figure 6. Erosion profile of cross section at varying positions on the rod (See Fig. 3).

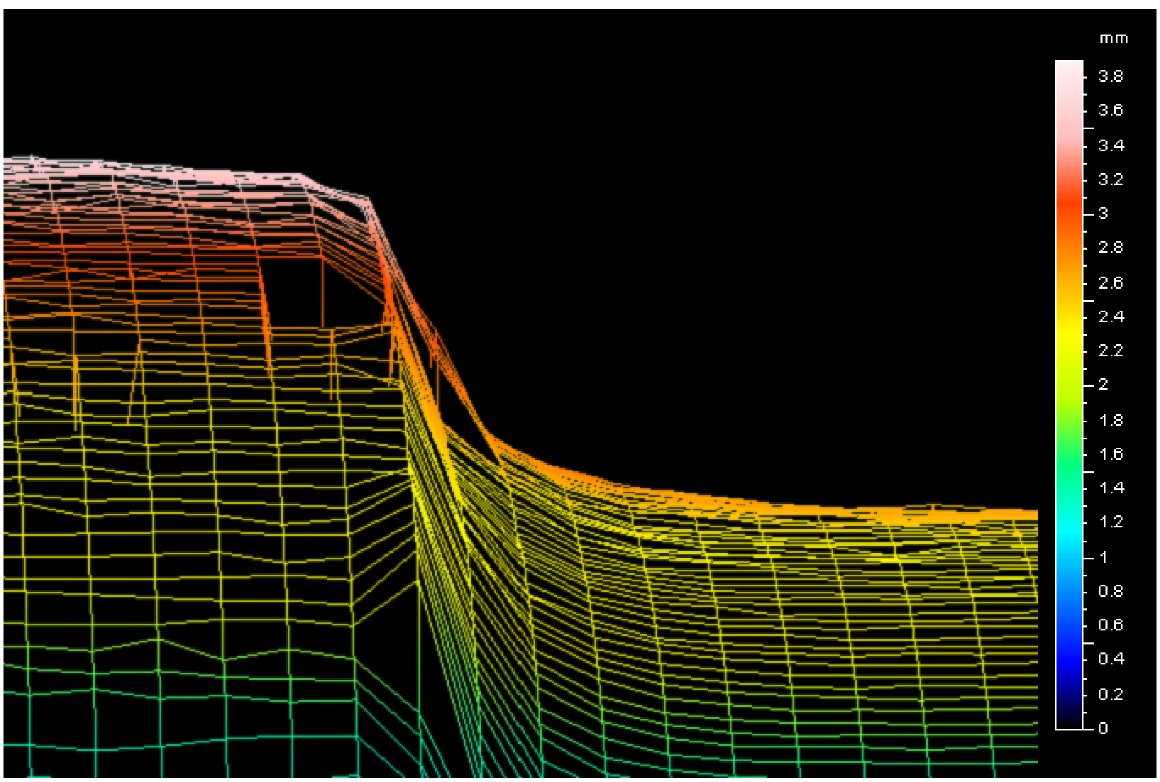

Figure 7. Transition are between eroded section and protected section of rod.

profile. Dependence curves with peaks further from 90 degrees result in sharper erosion profiles, such as the Yamamura aluminum line shown in Figure 10.

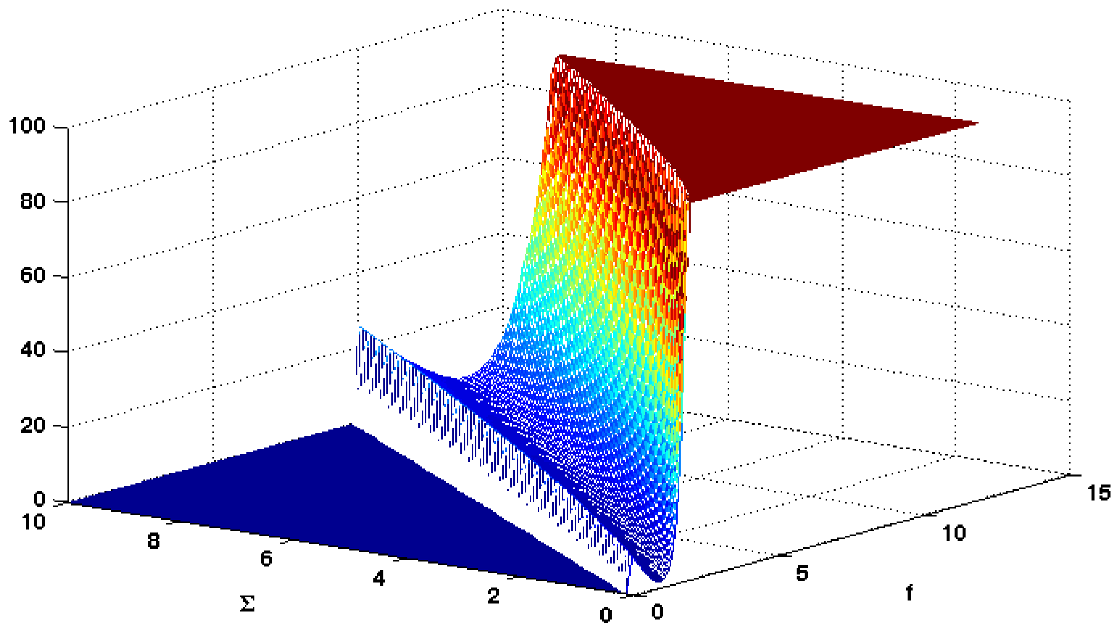

Figure 8. Surface mesh showing least squares fit of Yamamura constants.

Figure 10 shows that the calculated inputs for Yamamura match the experimental profile well, but neither the calculated constants, nor the experimental profile, match up to the profile resulting from the published values for aluminum. The unexpected erosion profile is likely due to the plasma source. The calculations performed assumed a mono-energetic, uniform, 200 eV plasma. The BHT-200 was thought to be an adequate approximation, but this may not have been correct.

Measurements of the BHT-200 plume[7,8] show three distinct populations: singly charged ions, doubly charged ions, and triply charged ions. These are in addition to electrons and neutral xenon particles. None of these species are mono-energetic, but are instead described by maxwellian distributions. Furthermore, Hall thrusters have beam divergence, collisions, and field effects that cause non axial velocity components to develop.

In future experiments it should be advantageous to use a more suitable ion source. Gridded ion thrusters have more columnated, mono-energetic beams and are being considered.

V. Coliseum Validation

A. Simulation Setup

The Coliseum code was used to simulate the erosion of a 0.25 in aluminum cylinder. The domain consisted of a 60x60x60 grid of 0.2 mm cells, for a total domain size of 12x12x12 mm. A 0.25 in cylinder consisting of 40 radial partitions and 20 axial partitions was inserted into the center of the domain. The simulation setup is shown in Figure 11. The cylinder extends vertically out of the domain to eliminate edge effects from the simulation.

The simulation was run for 10,000 timesteps of 2e-9 seconds. The erosion was calculated every 100 timesteps. Through use of the erosion rate multiplier, the total erosion time simulated was 72 hours. A plasma with properties given in Table 2 was injected from one side of the domain to replicate the plasma flux from the BHT-200 plume. Coliseum can simulate a BHT plume with reasonable accuracy,[8] however this study used a uniform plasma to replicate the idealized input conditions to the optimizer rather than the physical experimental plume.

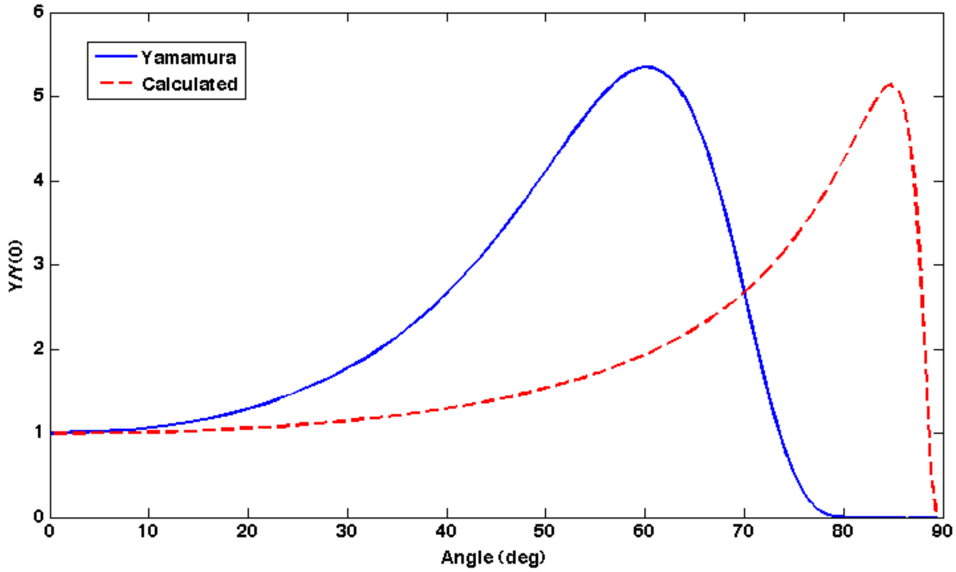

Figure 9. Angular dependence curves based on calculated constants and published Yamamura values.

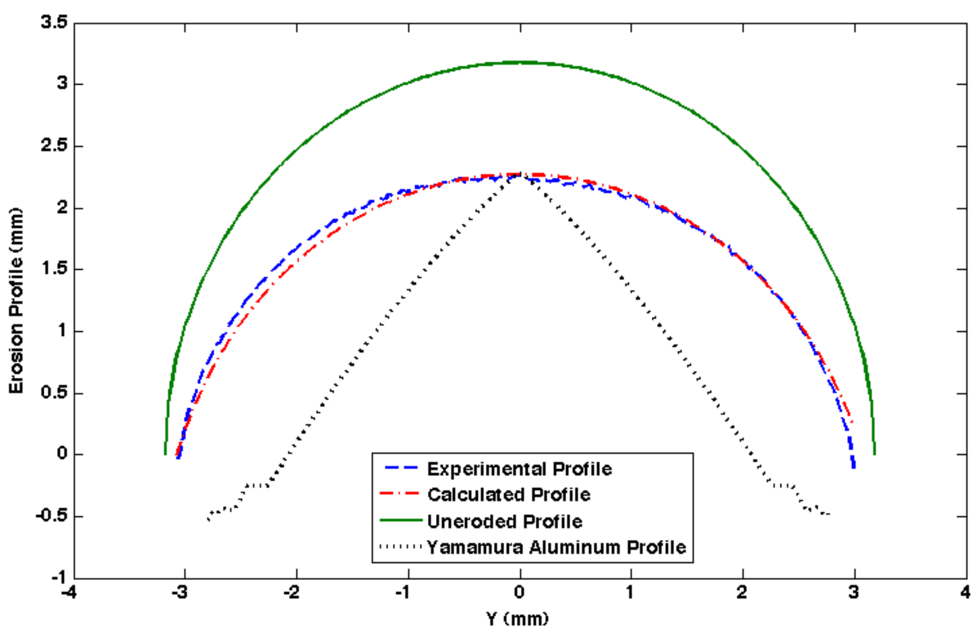

Figure 10. Erosion profiles compared with Yamamura value.

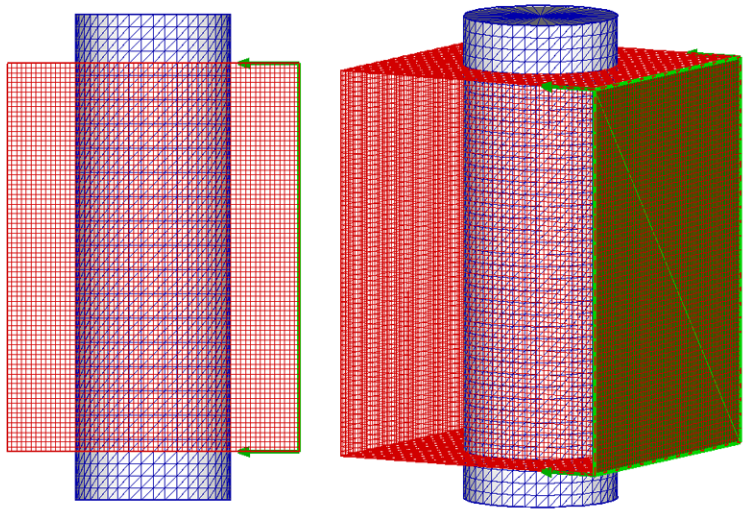

Figure 11. Simulation domain used by Coliseum. Particle source shown in green.

Plasma Parameters		
	Specie Parameters	
$s1$	Ion specie	Xe+
$s2$	Target specie	Al
$\dot{m}$	Mass flow rate	1E-6 (kg/s)
v	Ion exit velocity	16,800 (m/s)
T	Ion temperature	1,000 (K)

Table 2. Plasma source and material parameters used by Coliseum.

B. Results

Coliseum was used to further validate the erosion optimization routine. The erosion profile is shown in Figure 12 along with the experimental and optimizer profile. The Coliseum profile matches well with the profile from the optimizer. This makes sense as the calculated Yamamura values from the optimizer were used for the Coliseum calculation.

Similar to Figure 2, Figure 13 shows the eroded cylinder computed by Coliseum. This allows for a three dimensional view of the erosion profile rather than the two dimensional view from the optimizer. The area of transition between the eroded area and the area protected by the kapton tape is not resolved as well in the Coliseum simulation. This is because of the cell sizing of the surface mesh. Erosion of cells is split among that cells nodes based on distance from the impact point. Any node that is a member of a cell that is eroded will receive some erosion. It is therefore difficult to resolve effects smaller than one cell width, such as a taped edge. This effect can be mitigated by having a reduced cell size.

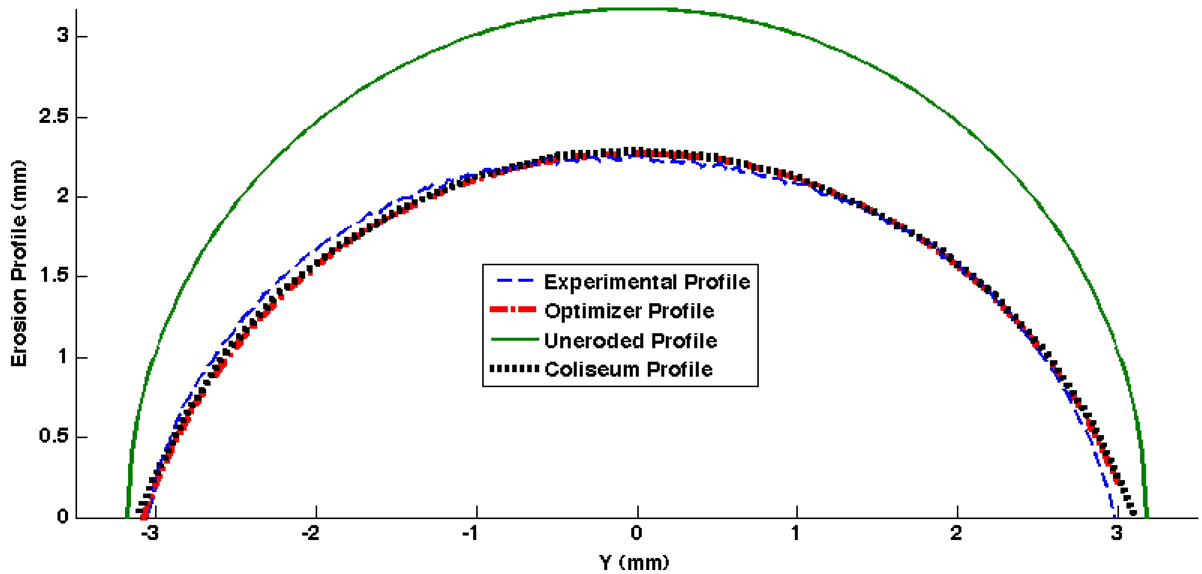

Figure 12. Coliseum erosion profiles compared with Yamamura profile and profile as calculated by optimizer along the center of the eroded area.

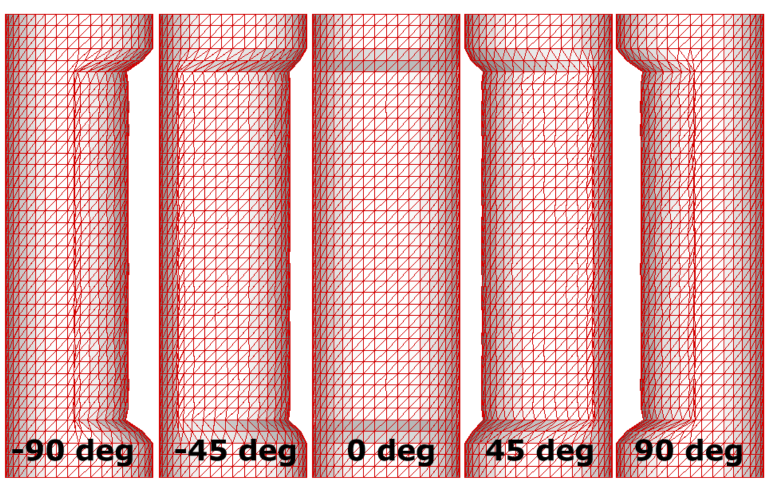

Figure 13. Eroded cylinder from Coliseum simulation.

VI. Future Work

This study presents a proof of concept for a method of measuring sputter yield angular dependence. Although the method and algorithms generated erosion profiles and dependence curves that matched the experimental data, the experimental data did not match published values. Additional erosion tests will be performed using a more uniform ion source, such as a gridded ion thruster. A detailed characterization of the plasma source will be required. Future improvements will also include attempting to match the rod potential with the plasma potential, and using a conductive tape instead of kapton.

Once the experimental setup is perfected, a variety of materials need to be tested including metals and nonmetals. Current plans are to test graphite and molybdenum. If this methodology proves accurate for well known materials, it can then be tested for largely unknown materials such as composites.

VII. Conclusion

Surface sputtering is a phenomenon that removes material from a surface by way of particle impingement. This effect is dependent on particle energy, incidence angle, and material properties. Current methods are limited to measuring sputtering at a single energy and angle of incidence resulting in many required experiments to fully characterize a given material. This work demonstrates a new technique to measure the angular sputter yield dependence for a given material in a single measurement.

An aluminum cylinder was exposed to a BHT-200 plume and allowed to erode for a period of 72 hours. The resulting profile was measured using an optical profilometer and compared to the initial, uneroded, shape. The erosion profile was fed into an optimization routine that used a least squares method to determine optimal constants for use in the Yamamura angular dependence function for sputter yields. Constants were calculated that resulted in a close match between the calculated erosion profile and the experimental profile.

Although the calculated profile matched well to the experiment, neither profile was consistent with published data. The likely cause of this is the ion source used. Hall effect thrusters do not emit a uniform plasma, as per the assumptions. Future studies should be conducted to determine if this method will obtain the correct dependence curves given a mono-energetic, columnated ion source.

Coliseum has a variety of plasma solving routines and now has a surface erosion routine. The erosion constants obtained from the optimizer can be used in Coliseum to model erosion of uncharacterized materials. This module can be used to model erosion on a variety of real world surfaces where erosion may be an issue. Particularly in cases with unique shapes, materials, and redeposition concerns, Coliseum will be a useful tool in predicting sputtering, redeposition, and surface erosion patterns.

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Calculating Sputter Rate Angular Dependence Using Optical Profilometry

Alex□□ Barrie

Advatech Pacific, Inc.

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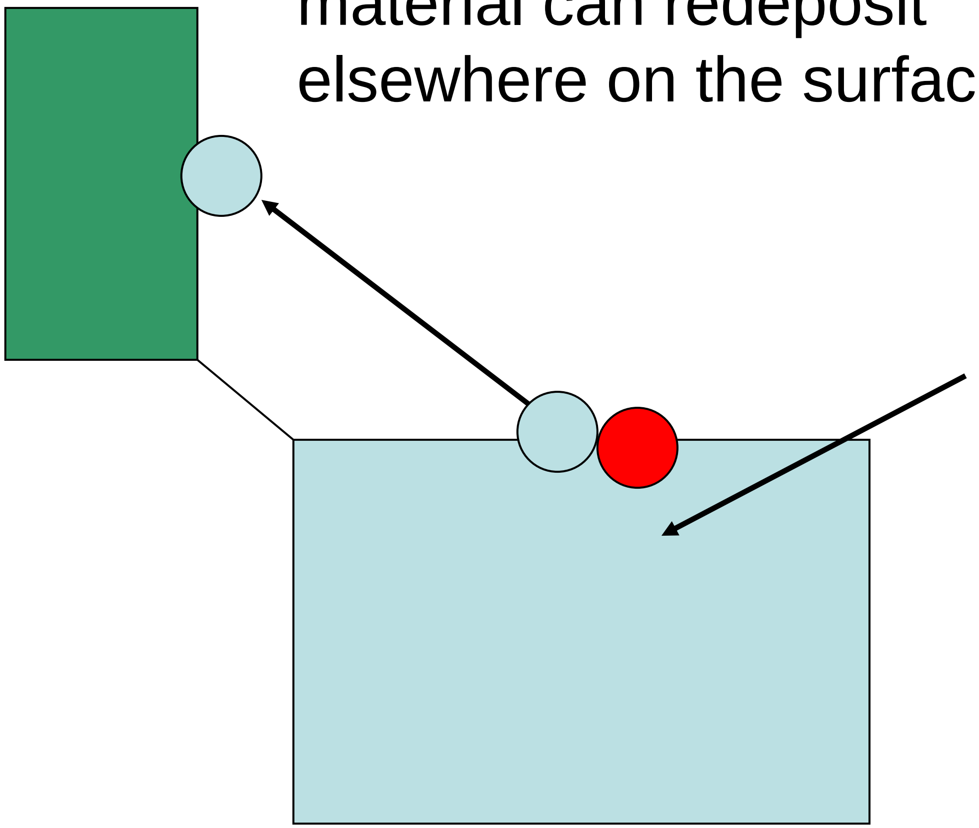
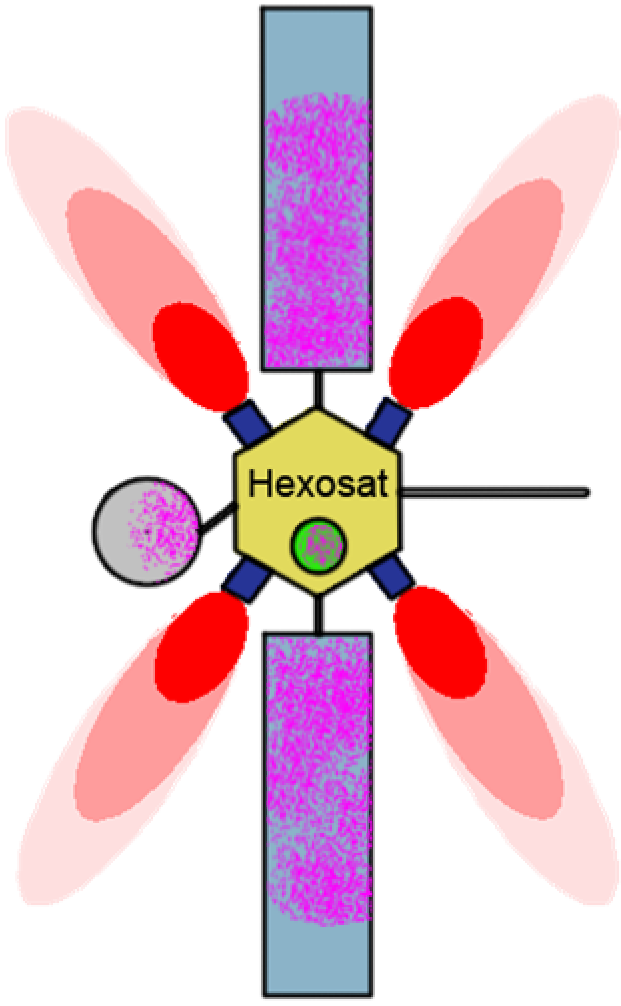
Sputtering

Particles impact a surface to sputter off material. This material can redeposit elsewhere on the surface





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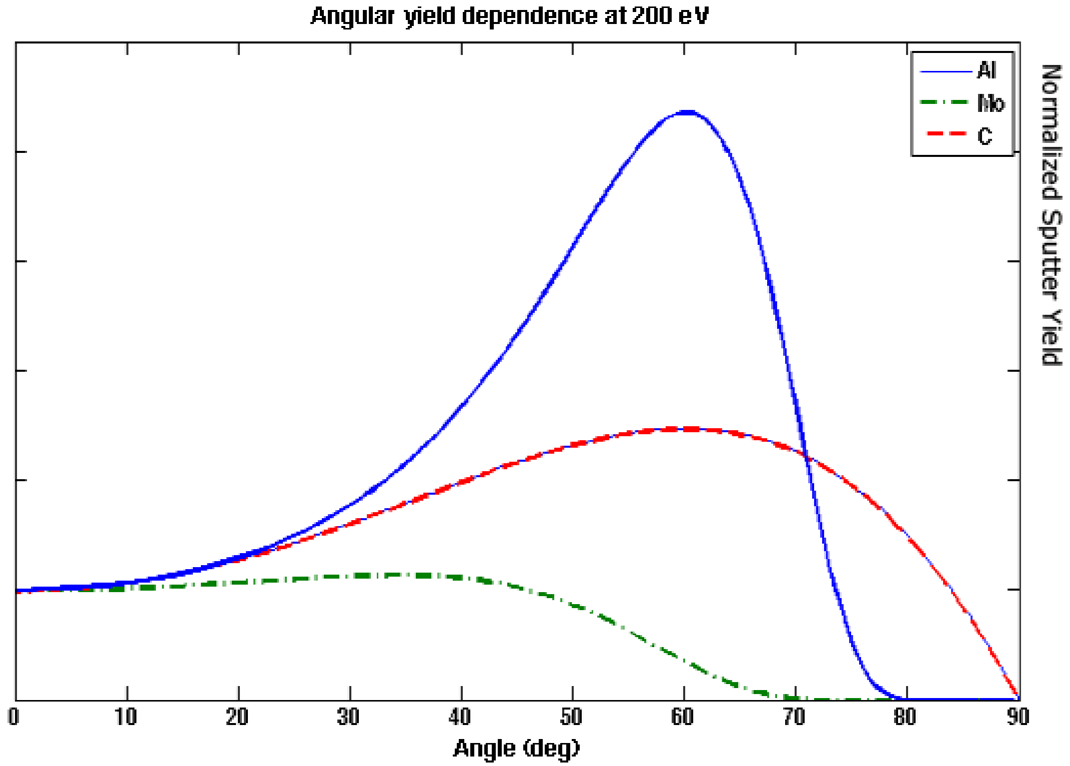
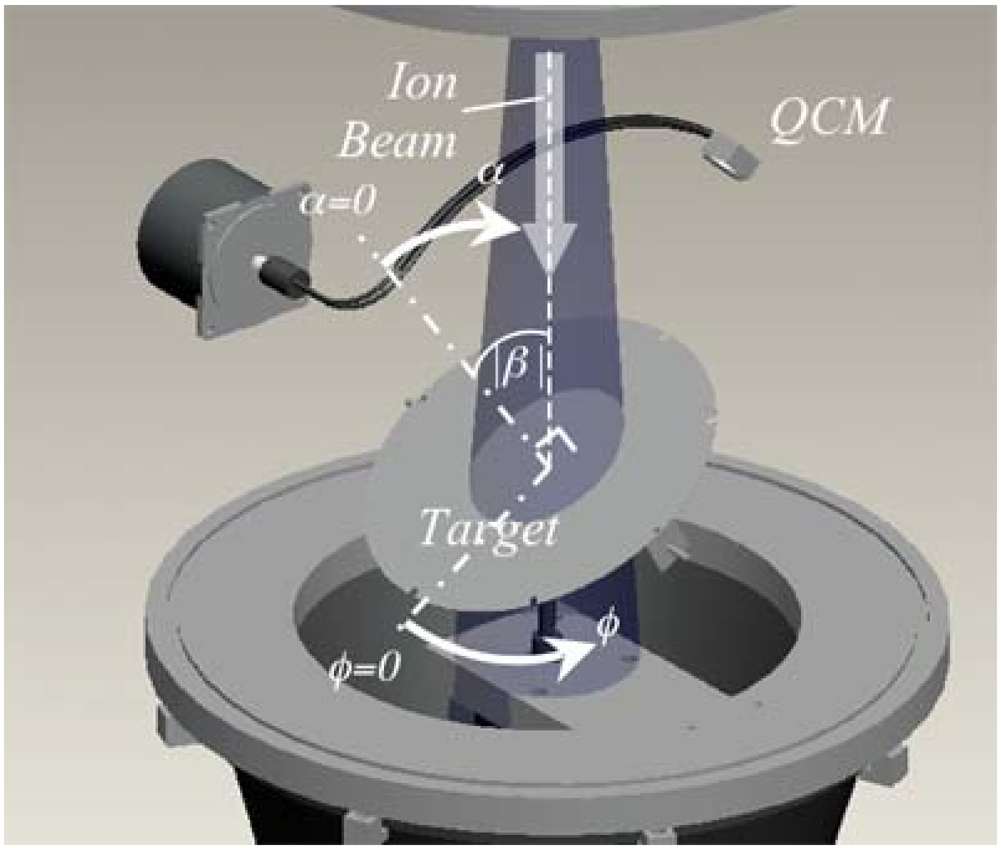
Angular Dependence



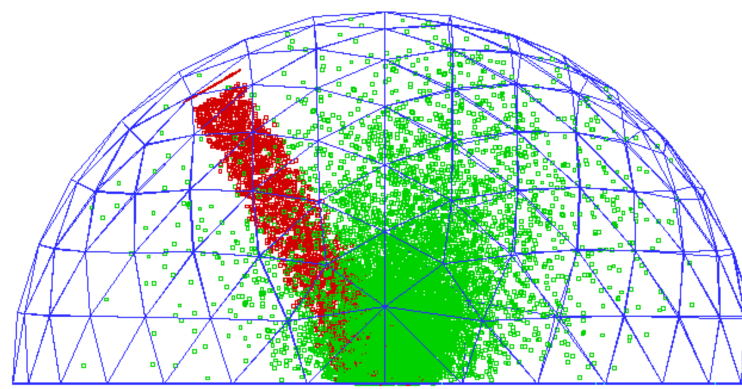
Sputter yields are dependent on both incident particle energy and impact angle

Current Method



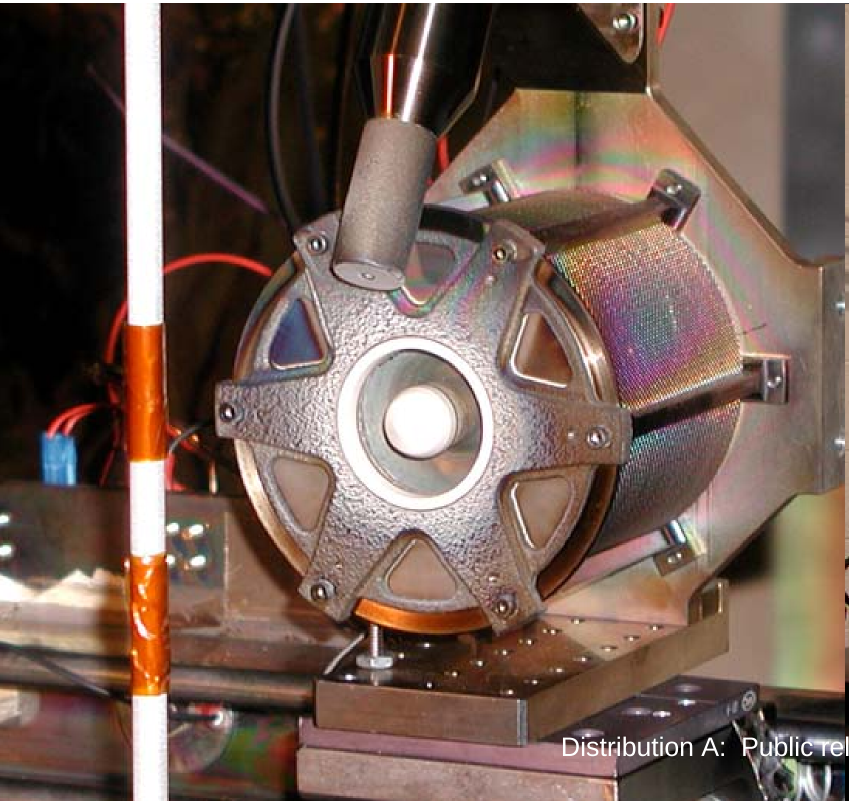
QCM image courtesy Colorado State Univ.

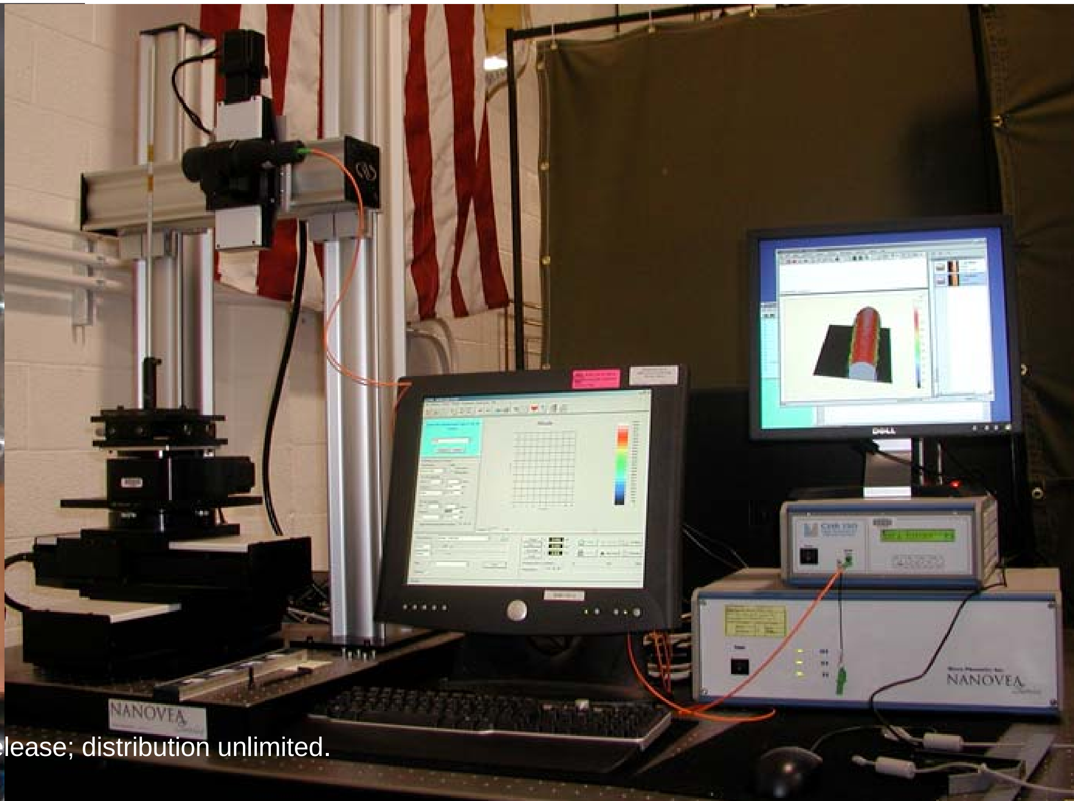
Current methods involve making a measurement for each incidence angle



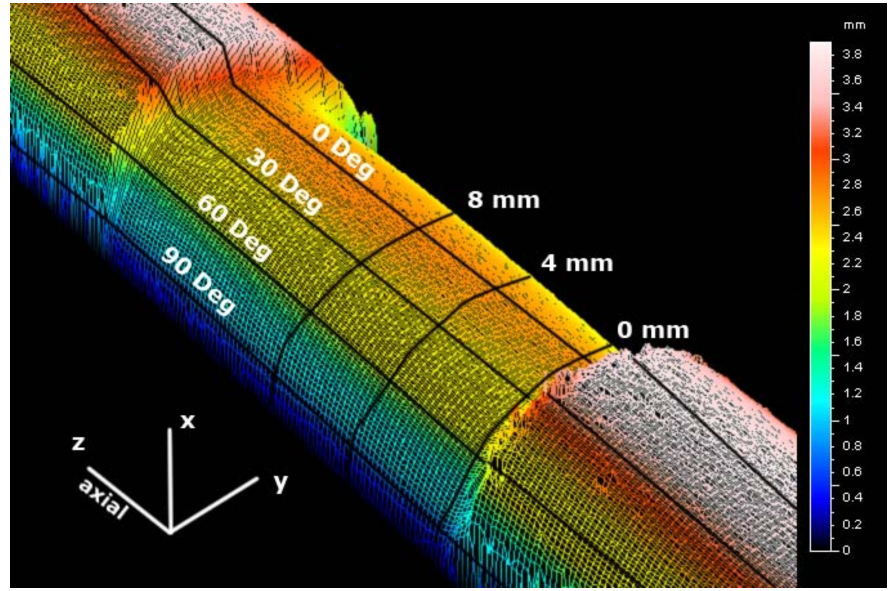
Experiment Details

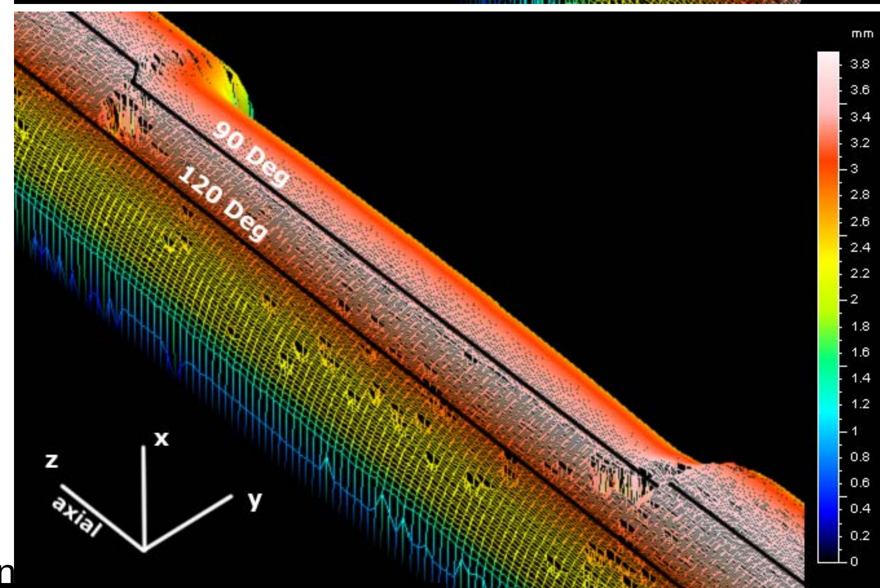
- Erode a 1/4” cylindrical rod using a BHT-200 plume for 72 hours
- Measure the resulting erosion profile
- Use an optimizer to determine an angular dependence profile that will generate the same profile



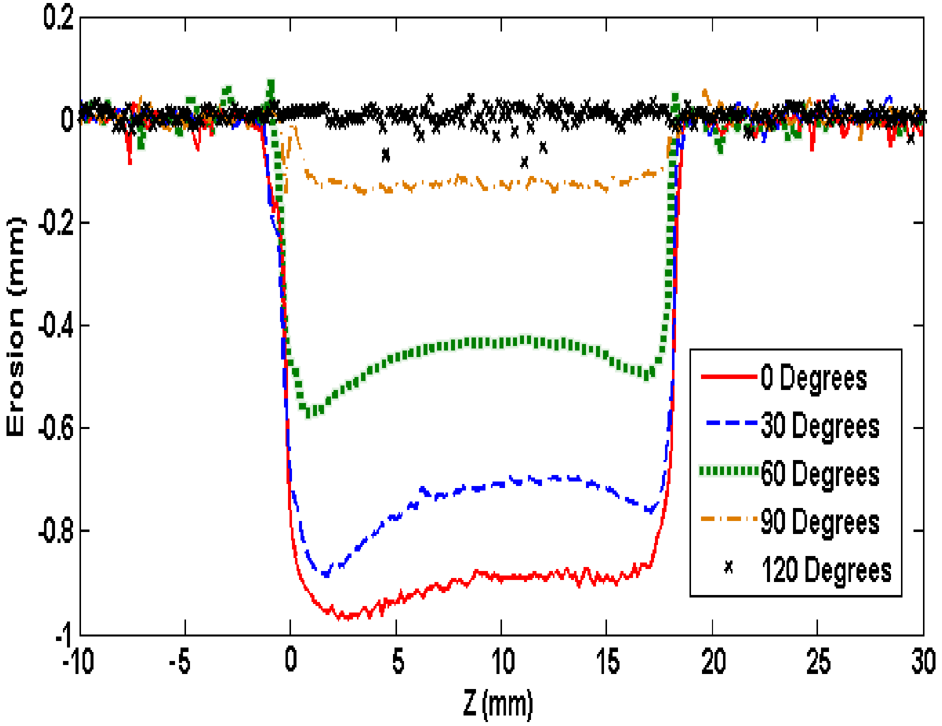


Erosion Measurements



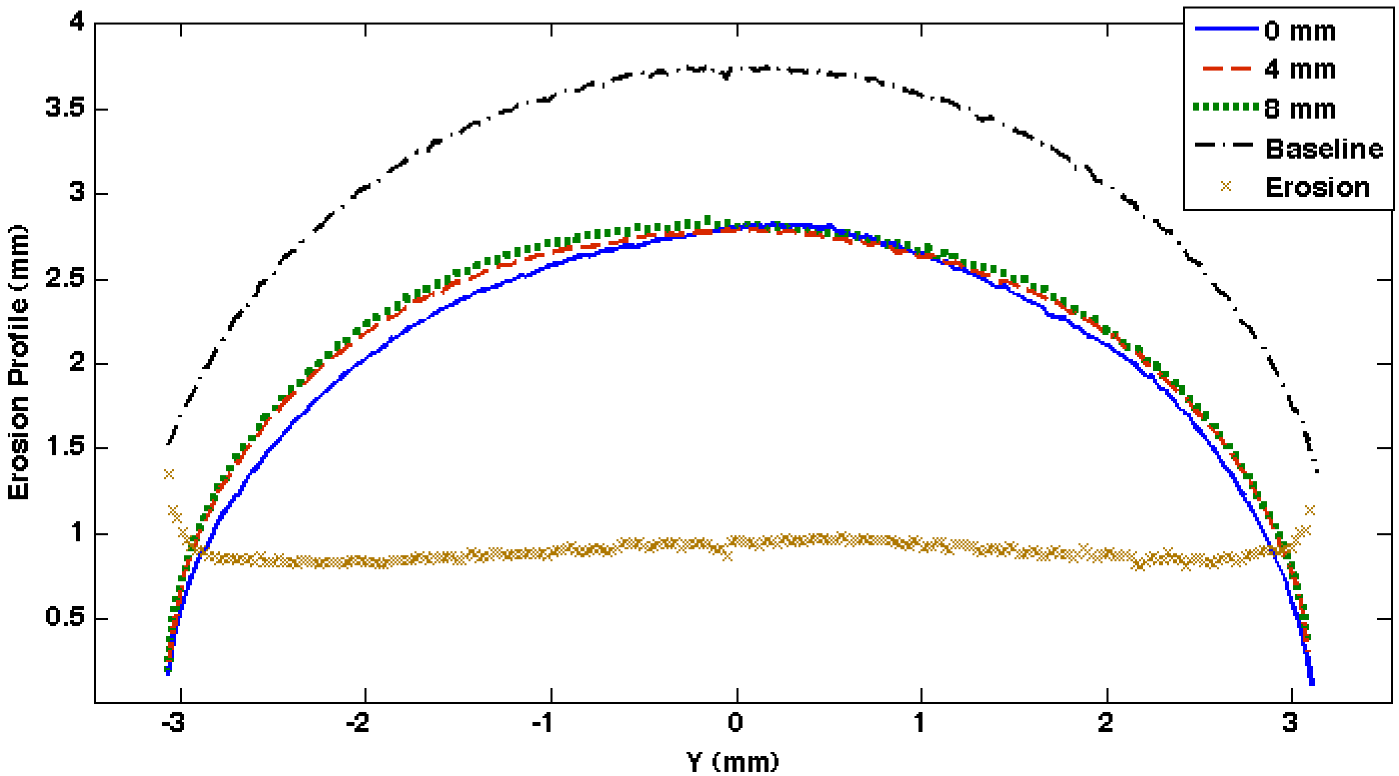


Vertical Erosion Profiles



- Lower erosion near center of channel
  - Charging effects from kapton tape
  - Ring shaped plume
- Higher erosion near left side of channel
  - Thruster slightly off center
  - Rod not perfectly vertical

Horizontal Erosion Profiles



- Slight nonuniformity along channel
- Total average erosion relatively constant

Yamamura

Normal Yield

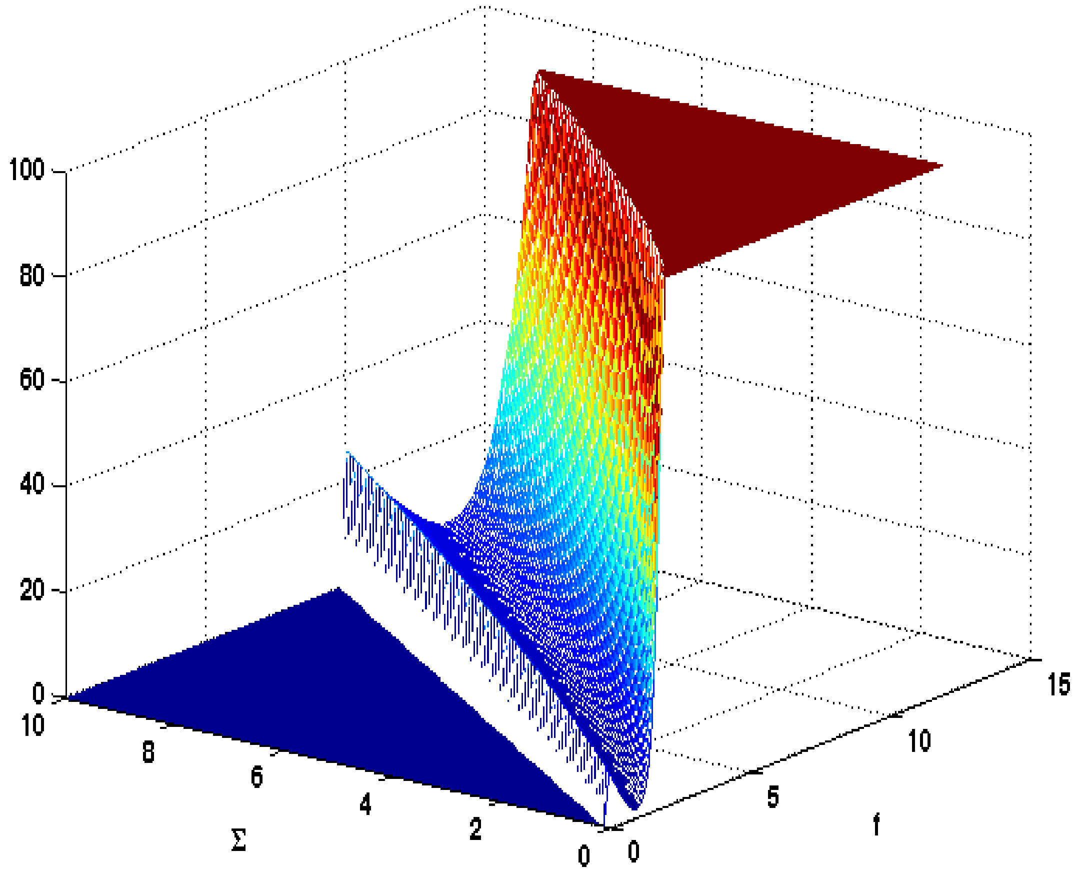
$$Y(E) = 0.042 \frac{Q(Z_2)\alpha^*(M_2/M_1)S_n(E)}{U_s(1+\Gamma k_e \varepsilon^{0.3})} \times \left[1 - \sqrt{\frac{E_{th}}{E}}\right]^s$$

Angular Dependence

$$Y(\theta) = Y(0)\cos^{-f}\theta e^{-\Sigma(\cos^{-1}\theta - 1)}$$

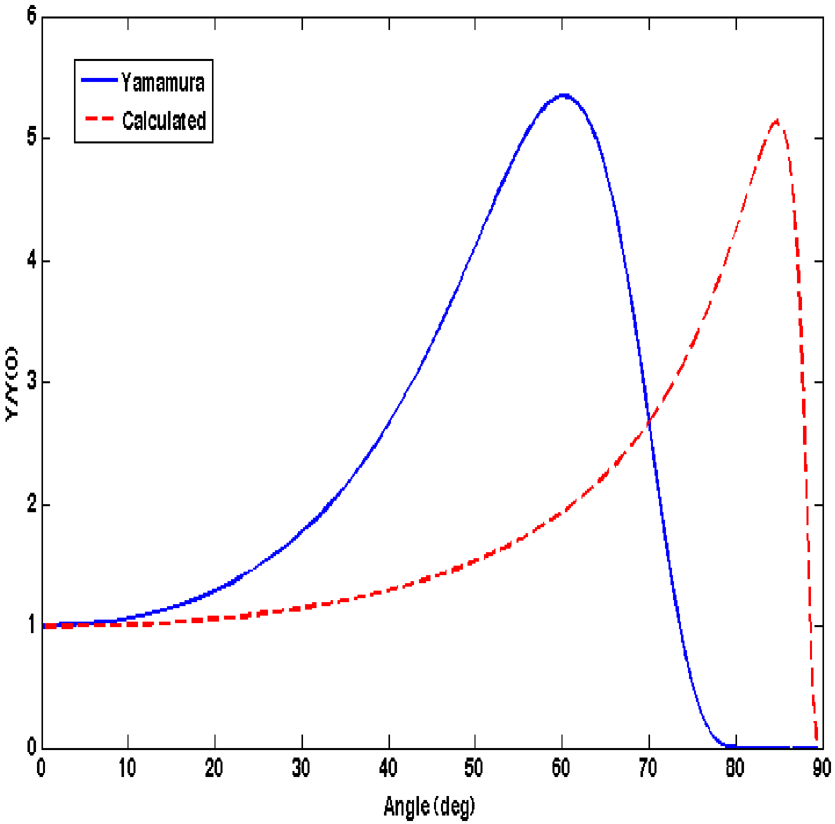
- Normal yield will be calculated based on normal erosion
- Angular dependence will be optimized along parameters f and Σ

Optimization



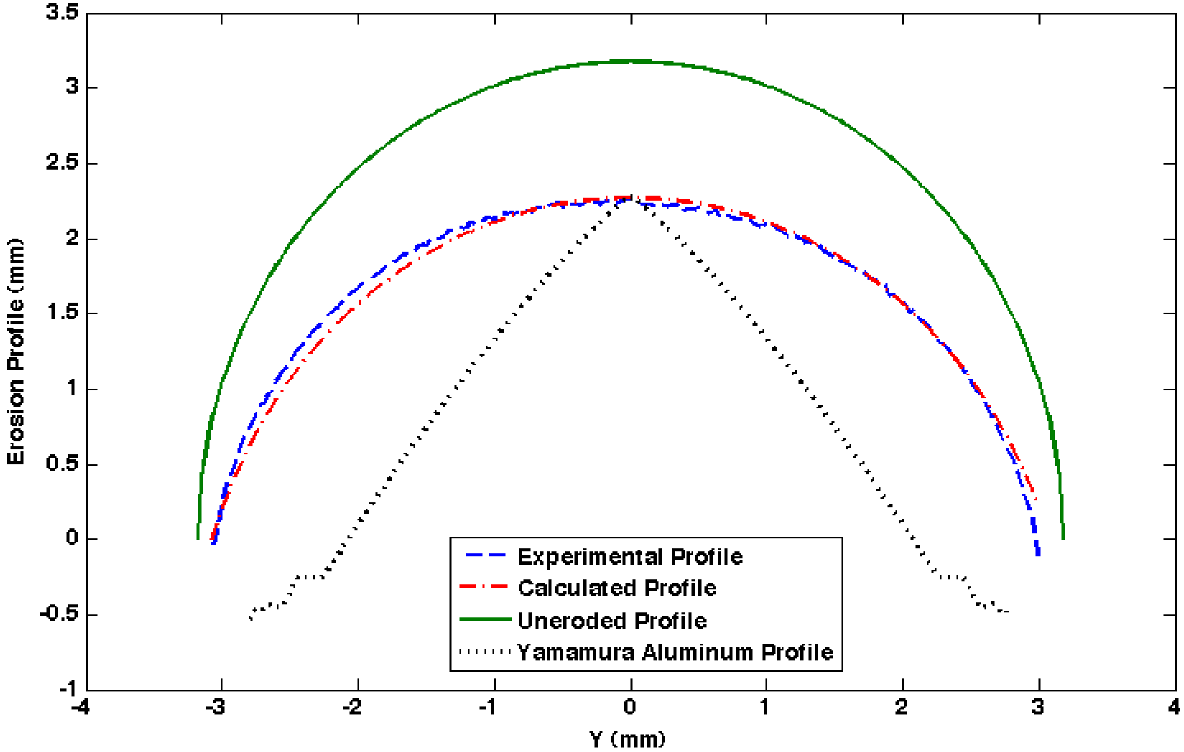
- Line of local minima represents values that match erosion profile near 0 and 90 degrees
- Position along line of local minima governs shape of angular dependence
- Absolute minimum found to be at Σ=0.1 and f=1.1
- Published values for aluminum are Σ=4.3 and f=8.6
  - This point lies on the line of local minima

Angular Dependence



- Calculated angular dependence has a similar magnitude, but at a higher angle
  - Low dependence for most of cylinder
  - High erosion near 90 degrees

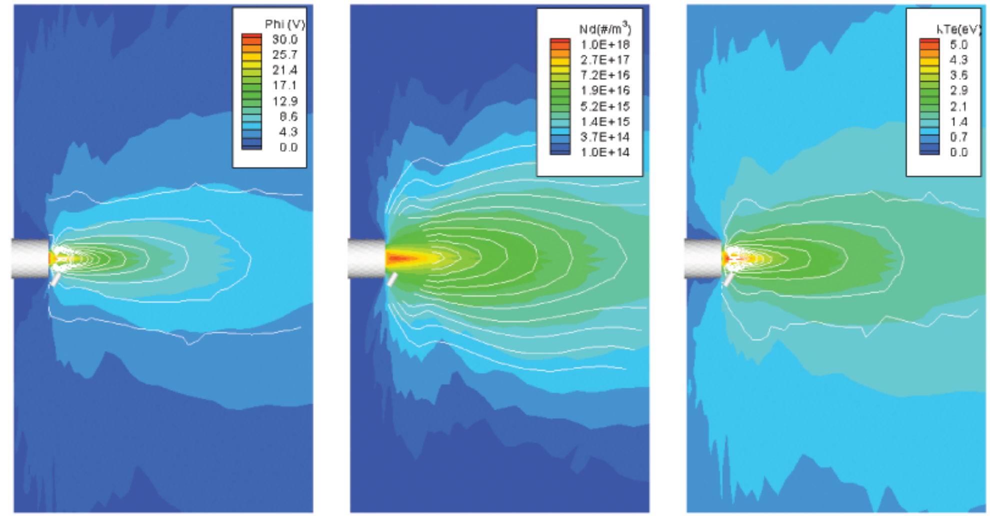
Surface Profile

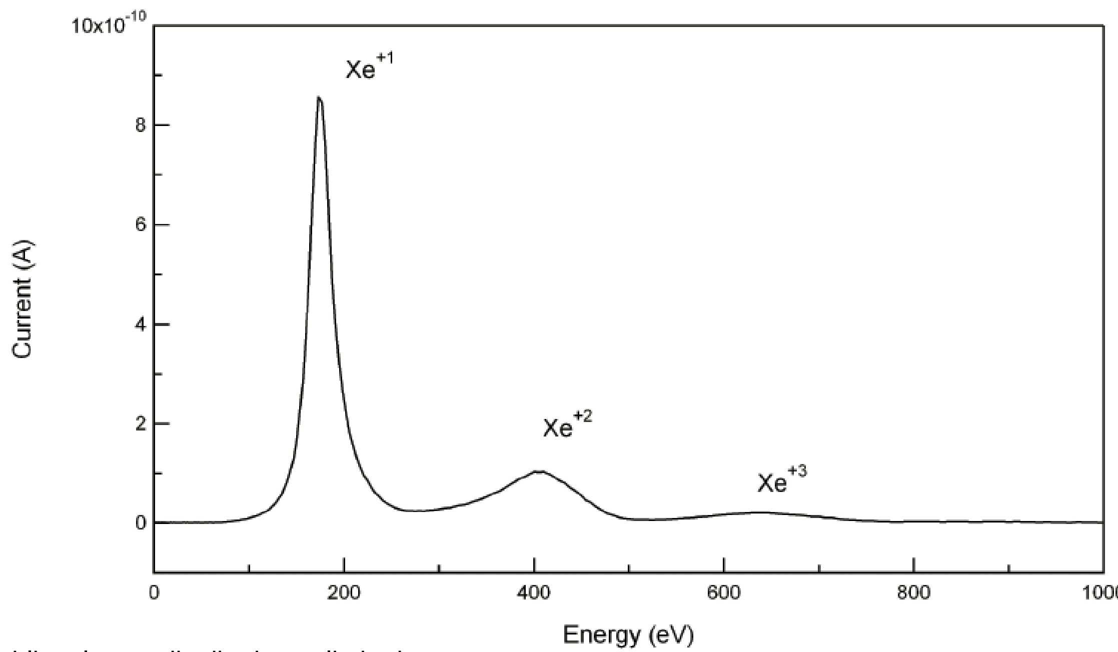


- Calculated profile lines up well with experimental profile, but neither profile matches the published Yamamura based curve
- Experimental profile must be flawed in some way

Error

- Error in experimental profile likely due to ion source
  - 200 eV mono-energetic, columnated source is assumed
  - Hall thrusters have several Maxwellian populations and have divergent plumes
- Use of a different ion source may alleviate this problem
  - Gridded ion thrusters are being considered





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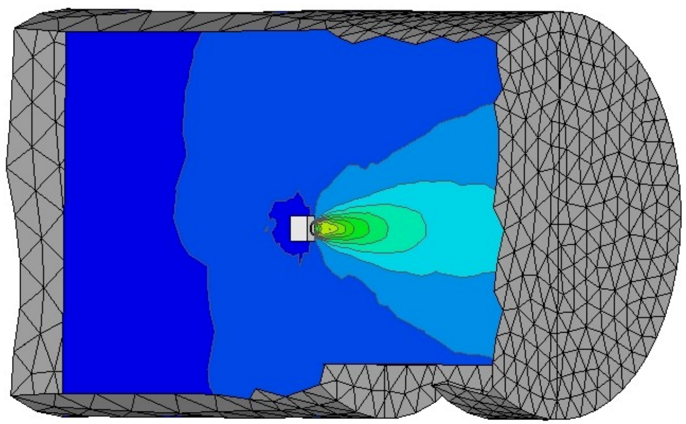
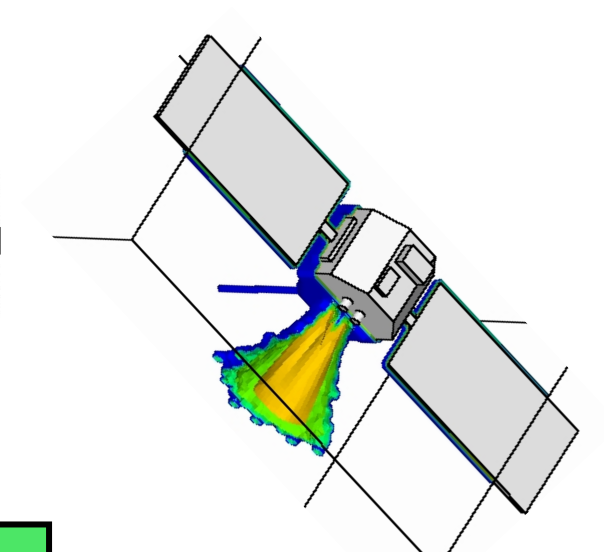
Distribution A: Public release; distribution unlimited.

Plots courtesy AFRL/PRSS

Coliseum Validation





Surface
- •Simulation mesh
- •Material specs

Particle Sources
- •Exp profile: LIF, j
- •HPHall, CHETC

Sputter Model
- •Lab measurements
- •Model, ***f(E,θ)***

Plasma Simulation:
- •RAY (sputtering / deposition)
- •PRESCRIBED_PLUME
- •AQUILA (Hybrid PIC-DSMC)
- •DRACO (Full/Hybrid PIC-DS/MCC)

Results
- •Plume properties
- •Surface erosion/deposit

Collisions
- •Cross-sections, literature
- •**Limited data**

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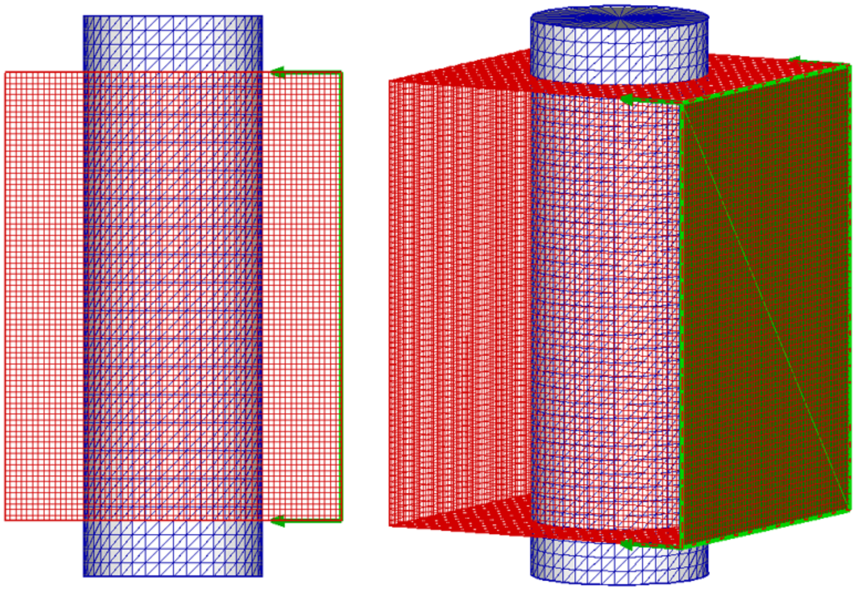
Coliseum Validation

- The Coliseum code was used to further validate the optimization routine
- The f, and Σ values were input to the Yamamura yield function
- A 200 eV columnated source was used
- Surface was allowed to erode for 72 hours

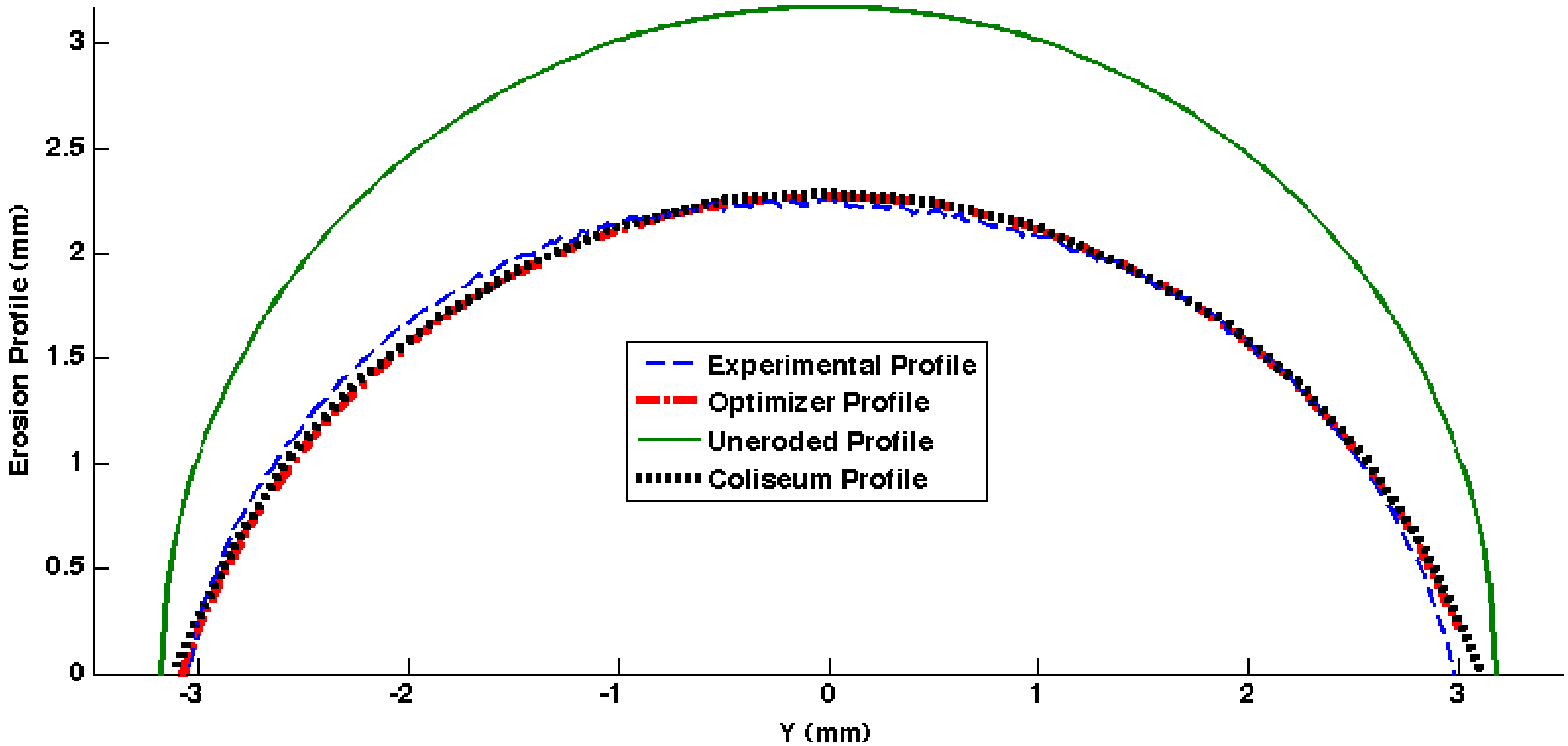


Coliseum Validation

Coliseum erosion profile over 72 hour period

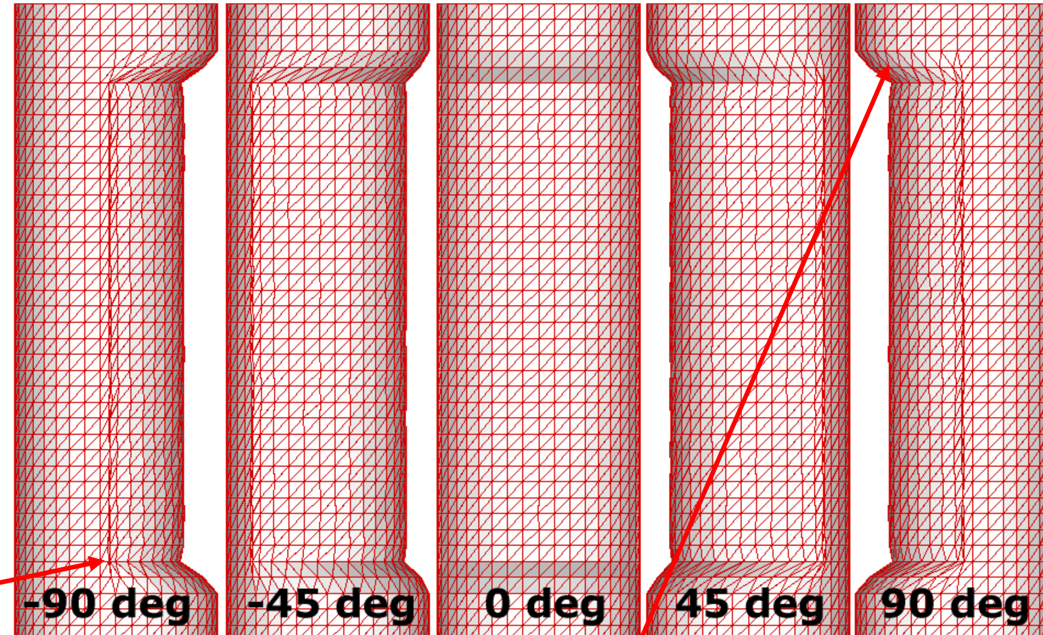
QuickTime™ and a
BMP decompressor
are needed to see this picture.

Coliseum Validation



- Coliseum profile matches with the optimizer profile
  - Based on inputs from optimizer
- Asymmetry of experimental case not captured

Coliseum Validation



- Erosion profile is similar
- Sharp edges are not captured
    - Effect of grid sizing
- Non-uniformity not captured
    - Effect of source model (flux)
        - Kapton tape, velocity distribution, source profile, etc.

Conclusions

- An optimizer was written to angular dependence of sputter yields with a single measurement
  - Optimizer functioned as expected, but experimental profile was not correct
  - Requires more mono-energetic beam
- Coliseum validation supports profile capabilities of optimizer

Future Work

- Perform profile experiment with better ion source
  - Monoenergetic
  - Columnated
- Test multiple materials
  - Graphite, molybdenum, quartz, etc.